



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 31, 2017 – 01:05 PM EST

PDB ID : 5H1S
EMDB ID: : EMD-9572
Title : Structure of the large subunit of the chloro-ribosome
Authors : Ahmed, T.; Yin, Z.; Bhushan, S.
Deposited on : 2016-10-11
Resolution : 3.50 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

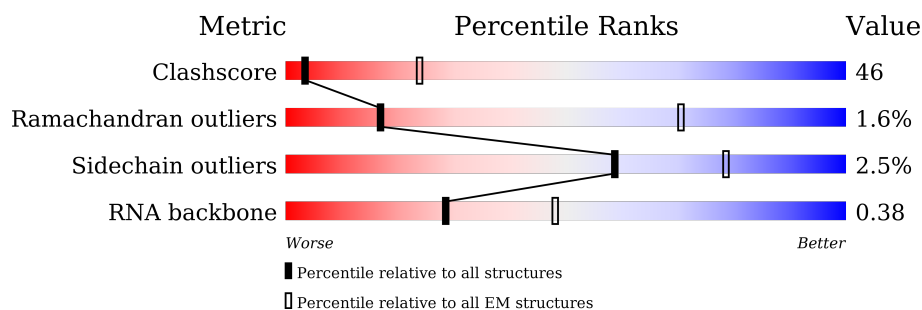
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



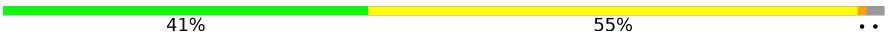
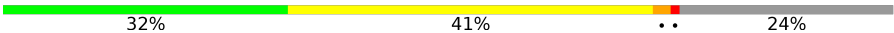

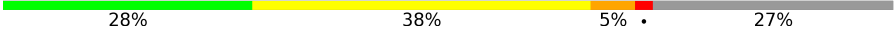
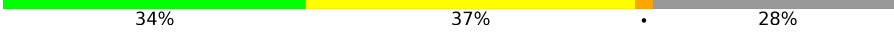
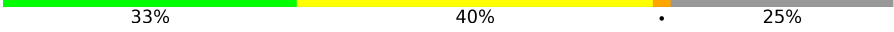


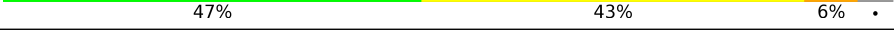



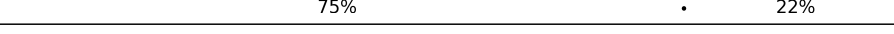
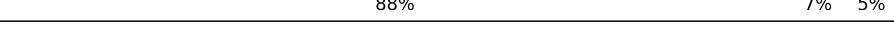

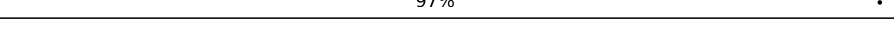



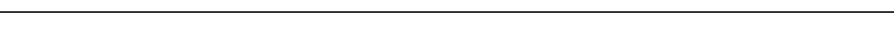




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	2810	29% 43% 27% .
2	C	106	9% 46% 37% . .
3	B	121	12% 43% 40% . .
4	L	191	36% 39% . . 23%
5	M	121	54% 46%
6	N	192	31% 51% 9% . 8%
7	O	135	44% 54% . .
8	P	116	57% 43%

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Mol	Chain	Length	Quality of chain
9	Q	123	
10	R	156	
11	S	127	
12	T	201	
13	U	199	
14	V	122	
15	W	145	
16	X	137	
17	Y	77	
18	Z	109	
19	E	271	
20	b	56	
21	c	65	
22	d	60	
23	e	73	
24	f	37	
25	F	221	
26	G	243	
27	H	220	
28	I	182	
29	J	155	
30	g	142	
31	a	94	
32	h	116	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 90825 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2799	Total	C	N	O	P	0	0
			60117	26819	11134	19365	2799		

- Molecule 2 is a RNA chain called Spinach chloroplast 4.5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	102	Total	C	N	O	P	0	0
			2187	977	403	705	102		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	117	Total	C	N	O	P	0	0
			2500	1116	452	815	117		

- Molecule 4 is a protein called 50S ribosomal protein L13, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	147	Total	C	N	O	S	0	0
			1184	754	225	202	3		

- Molecule 5 is a protein called 50S ribosomal protein L14, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	121	Total	C	N	O	S	0	0
			942	588	179	170	5		

- Molecule 6 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	177	Total	C	N	O	S	0	0
			1342	836	264	236	6		

- Molecule 7 is a protein called 50S ribosomal protein L16, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	134	Total	C	N	O	S	0	0
			1067	672	217	173	5		

- Molecule 8 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	116	Total	C	N	O	S	0	0
			944	592	193	155	4		

- Molecule 9 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	120	Total	C	N	O	S	0	0
			947	589	183	170	5		

- Molecule 10 is a protein called 50S ribosomal protein L19, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	R	118	Total	C	N	O	S	0	0
			953	610	186	156	1		

- Molecule 11 is a protein called 50S ribosomal protein L20, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	115	Total	C	N	O	S	0	0
			996	633	208	153	2		

- Molecule 12 is a protein called 50S ribosomal protein L21, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	T	147	Total	C	N	O	0	0
			1171	759	202	210		

- Molecule 13 is a protein called 50S ribosomal protein L22, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	144	Total	C	N	O	S	0	0
			1149	731	210	200	8		

- Molecule 14 is a protein called 50S ribosomal protein L23, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	92	Total	C	N	O	S	0	0
			740	477	129	132	2		

- Molecule 15 is a protein called 50S ribosomal protein L24, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	124	Total	C	N	O	S	0	0
			993	624	187	180	2		

- Molecule 16 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	100	Total	C	N	O	S	0	0
			810	511	159	140			

- Molecule 17 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	74	Total	C	N	O	S	0	0
			605	385	121	98	1		

- Molecule 18 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	90	Total	C	N	O	S	0	0
			754	470	150	131	3		

- Molecule 19 is a protein called 50S ribosomal protein L2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	E	247	Total	C	N	O	S	0	0
			1904	1181	390	327	6		

- Molecule 20 is a protein called 50S ribosomal protein L32, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	46	Total	C	N	O	S	0	0
			378	250	70	58			

- Molecule 21 is a protein called 50S ribosomal protein L33, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	c	51	Total	C	N	O	S	0	0
			415	258	83	70	4		

- Molecule 22 is a protein called 50S ribosomal protein L34, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	d	57	Total	C	N	O	S	0	0
			445	268	103	71	3		

- Molecule 23 is a protein called 50S ribosomal protein L35, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	e	69	Total	C	N	O	S	0	0
			563	353	119	90	1		

- Molecule 24 is a protein called 50S ribosomal protein L36, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	f	37	Total	C	N	O	S	0	0
			304	186	70	44	4		

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	F	212	Total	C	N	O	S	0	0
			1620	1025	295	289	11		

- Molecule 26 is a protein called 50S ribosomal protein L4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	G	210	Total	C	N	O	S	0	0
			1655	1052	308	292	3		

- Molecule 27 is a protein called 50S ribosomal protein L5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	H	175	Total	C	N	O	S	0	0
			1351	862	233	248	8		

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	I	173	Total	C	N	O	S	0	0
			1353	855	249	245	4		

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	J	53	Total	C	N	O	S	0	0
			423	280	74	68	1		

- Molecule 30 is a protein called 50S ribosomal protein 5 alpha, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	43	Total	C	N	O	S	0	0
			345	218	65	59	3		

- Molecule 31 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	38	Total	C	N	O	S	0	0
			300	187	49	62	2		

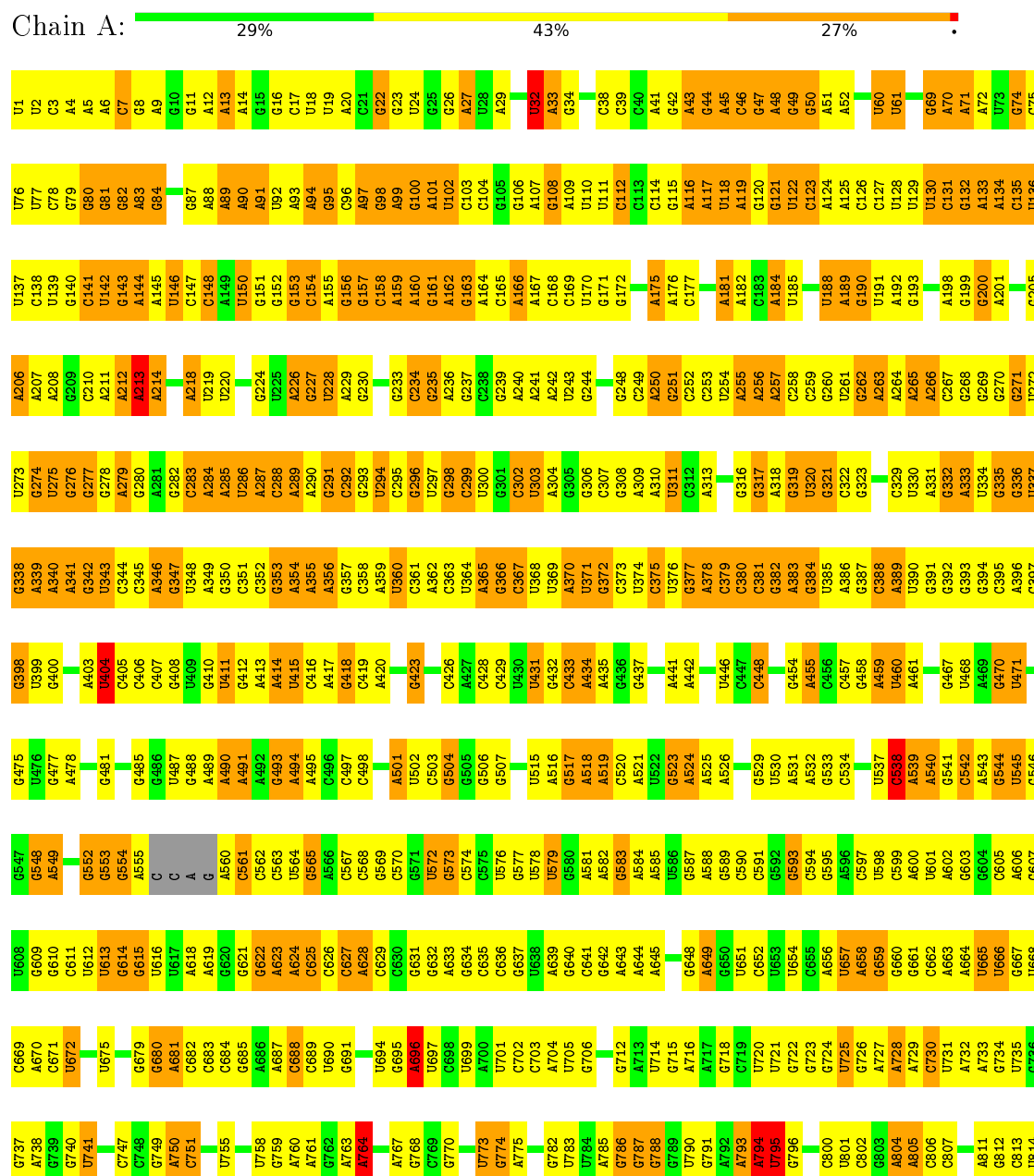
- Molecule 32 is a protein called 50S ribosomal protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	h	46	Total	C	N	O	S	0	0
			368	237	71	59	1		

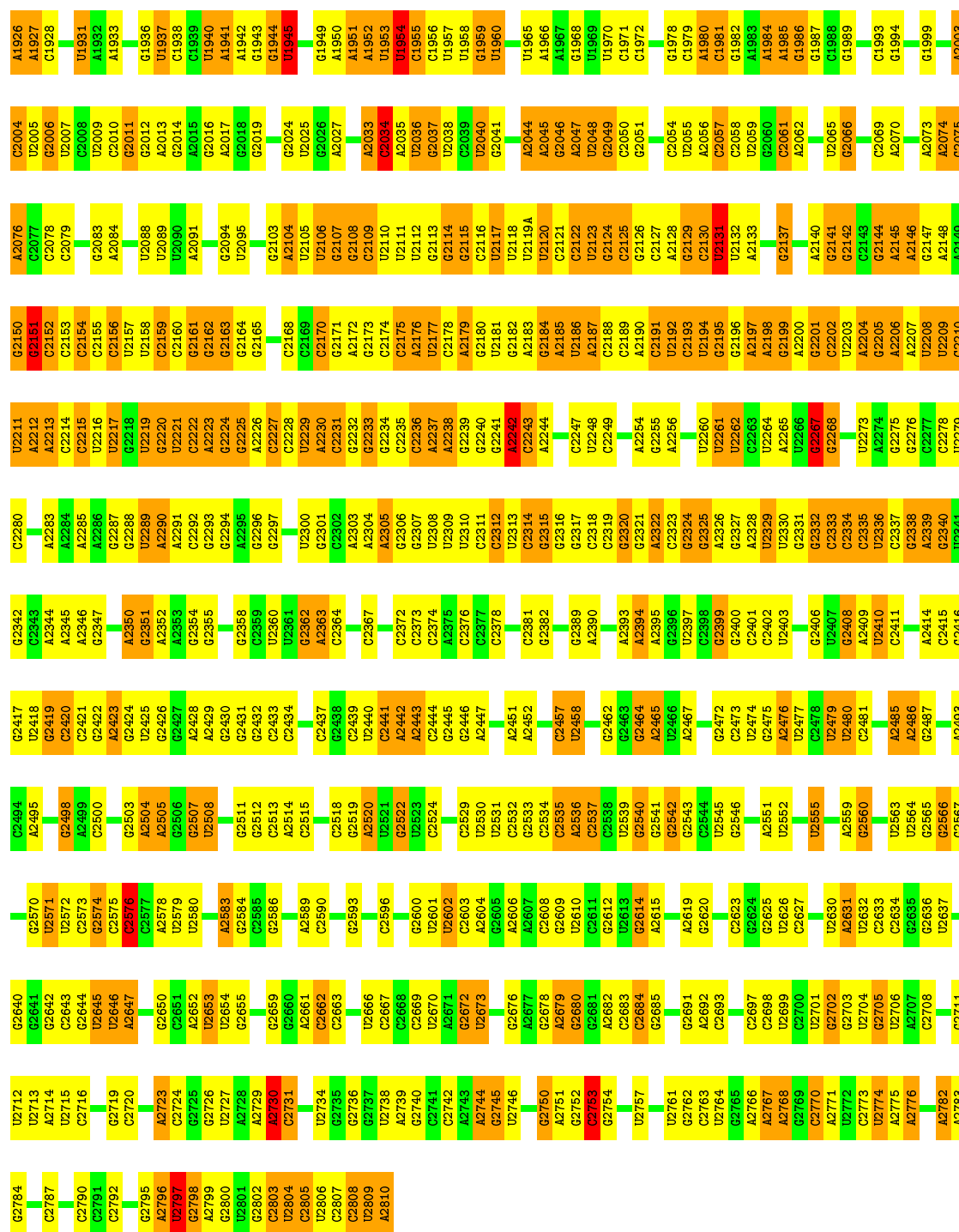
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

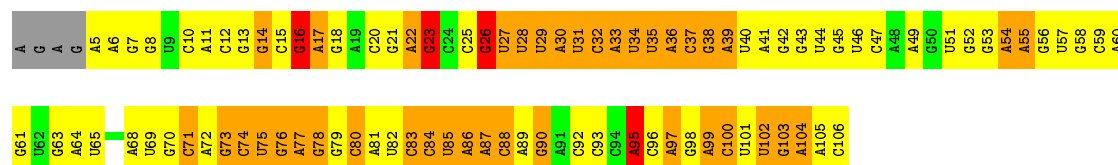
• Molecule 1: 23S rRNA



C1947	C1848	A1849	U1850	U1851	C1852	C1853	A1857	A1858	G1859	U1860	U1861	G1866	A1867	A1868	U1869	U1870	U1871	G1872	G1873	G1874	U1875	A1876	C1877	C1878	U1879	A1880	A1881	U1882	A1883	C1884	A1885	C1886	A1887	G1888	G1889	A1890	A1891	C1892	G1895	G1896	C1897	G1898	C1899	A1900	A1901	C1902	G1903	A1904	C1905	G1906	C1907	A1908	A1909	G1910	C1911	G1912	A1913	C1914	A1915	C1916	G1917	G1920	G1921	C1842
C1781	C1782	A1783	G1709	G1710	C1711	G1786	U1789	U1793	A1794	A1795	A1796	A1797	G1798	A1799	G1723	G1730	G1731	G1732	G1733	G1734	G1735	U1736	U1737	G1808	G1809	C1810	A1811	A1812	A1813	G1814	U1815	C1816	G1817	U1818	A1819	A1820	G1821	A1822	C1823	C1824	A1825	U1826	G1827	U1828	A1829	U1830	G1831	G1832	G1833	G1834	A1914	A1915	C1916	G1917	G1920	G1921	C1842							
A1705	C1706	G1707	G1708	C1709	C1710	C1711	A1712	A1713	A1714	A1715	A1716	A1717	G1718	G1723	G1730	G1731	G1732	G1733	G1734	G1735	U1736	U1737	G1808	G1809	C1810	A1811	A1812	A1813	G1814	U1815	C1816	G1817	U1818	A1819	A1820	G1821	A1822	C1823	C1824	A1825	U1826	G1827	U1828	A1829	U1830	G1831	G1832	G1833	G1834	A1914	A1915	C1916	G1917	G1920	G1921	C1842								
G1630	G1631	U1632	A1633	C1634	C1635	U1636	G1637	G1643	G1644	A1645	A1646	C1647	C1648	C1649	A1650	C1651	A1652	C1653	C1654	C1655	A1662	G1663	U1664	U1665	G1666	U1667	A1668	A1669	A1670	A1671	U1672	A1673	C1674	C1675	U1676	C1682	G1683	C1684	G1687	A1688	C1689	A1690	A1691	C1692	U1693	C1694	U1697	A1698	A1699	A1700	A1625	A1626	G1702	C1703	A1704									
C1570	G1571	C1572	C1573	G1574	C1575	U1576	G1577	A1578	G1579	U1580	U1581	A1582	A1583	C1584	C1585	A1586	A1587	U1588	C1589	C1590	A1591	A1592	U1593	A1594	C1595	U1596	C1597	C1598	C1599	A1600	G1601	C1602	A1603	A1604	A1605	A1606	G1607	C1608	U1609	C1610	G1611	A1612	A1613	C1614	G1615	A1616	C1617	C1618	U1619	U1620	C1621	A1622	A1623	C1624	A1625	A1626	G1702	A1628	G1629					
G1507	U	U	U	U	U	U	A	G1515	G1516	G1517	U1518	A1519	A1520	G1521	A1522	A1523	G1524	G1525	C1526	U1527	U1528	A1529	C1530	A1531	G1532	A1533	A1534	A1535	A1536	U1537	G1538	C1539	C1540	U1541	C1542	G1543	A1544	G1545	C1546	C1547	A1548	A1549	U1550	G1551	U1552	U1553	C1554	G1555	A1556	G1557	U1558	A1559	A1562	G1566	C1567	C1568	A1569							
C1443	A1444	A1445	A1446	A1448	C1449	G1450	G1451	A1452	G1453	A1454	G1457	C1458	U1459	A1460	G1461	G1462	U1463	U1464	A1465	G1466	C1467	C1468	C1469	A1470	A1471	A1472	G1473	A1474	C1397	U1398	A1399	U1400	U1401	U1406	C1407	C1408	G1482	G1483	G1484	U1485	U1486	C1487	A1488	A1489	C1493	G1494	C1495	A1496	A1497	G1498	G1499	U1500	G1501	A1502	C1503	C1504	C1505	U1506	U1438					
G1277	U1278	G1281	C1282	U1283	U1284	G1285	A1286	G1287	U1288	A1289	A1290	C1291	G1292	C1293	A1294	A1295	A1296	C1297	A1298	U1299	A1305	A1306	A1307	U1308	U1309	C1310	C1311	A1312	A1313	G1314	G1315	C1316	C1317	C1318	C1319	G1320	U1321	A1322	A1323	G1332	U1333	C1334	C1335	C1336	U1337	C1338	C1341	A1342	A1343	U1344	U1345	U1346	U1347	C1348	G1349									
A1204	G1207	G1208	U1209	U1210	G1211	U1219	U1220	G1224	G1225	U1226	U1227	G1231	A1232	G1233	A1234	A1235	G1236	G1237	G1238	C1239	G1240	U1241	G1242	U1243	U1244	U1245	G1246	A1247	G1248	G1251	C1252	G1253	U1254	U1255	G1256	G1257	A1258	C1259	G1260	A1261	A1262	G1263	C1264	G1265	G1266	A1267	A1268	C1269	A1270	A1271	A1272	G1273	A1274	U1275	U1276									
C1141	G1142	U1143	U1144	U1145	U1146	U1147	G1150	G1153	A1154	A1155	G1156	A1157	U1158	G1159	A1160	A1161	C1162	G1163	G1164	G1165	G1166	G1167	U1168	A1169	A1170	G1171	C1172	G1173	U1174	U1175	U1176	U1177	G1178	C1179	C1180	G1181	A1182	A1183	G1184	C1185	U1186	G1187	U1188	G1189	A1192	U1193	G1194	U1195	A1196	A1197	C1198	A1199	A1200	A1201	A1202	C1203								
U1069	G1070	C1071	A1072	A1073	A1074	G1075	A1076	C1077	A1078	G1079	C1080	A1081	A1082	G1083	U1084	A1085	G1086	G1087	U1088	U1089	G1091	A1097	A1098	G1099	C1103	C1104	U1107	C1108	U1109	U1110	G1111	G1112	A1113	G1114	G1115	A1116	G1117	U1118	G1119	U1122	U1125	C1130	A1131	C1132	U1133	U1134	C1135	A1136	C1137	G1138	A1139	G1140												
G1005	G1006	A1007	A1008	A1009	C1010	A1011	G1012	C1013	G1016	G1017	A1018	U1019	G1020	A1021	C1022	C1023	A1024	G1025	A1028	A1029	U1030	G1031	C1032	C1033	C1034	C1035	U1036	A1037	A1038	U1039	U1040	G1041	A1042	G1043	C1044	G1045	C1046	U1047	C1048	A1049	G1050	U1051	A1052	A1053	U1054	A1055	A1056	A1057	A1060	G1061	U1062	U1063	A1064	G1065	G1066									
U942	C943	C944	A945	A946	A947	U948	A949	A950	C951	G952	G953	A954	G955	G956	C957	C958	A959	A960	G961	U962	U963	G964	G965	G966	C967	C968	A969	G970	A971	G972	A973	A974	A975	G976	G977	A978	U979	G980	G981	G982	G983	G984	A985	U986	A987	A988	U989	A992	A994	G997	U998	C999	G1000	A1001	G1002	A1003	G1004							
U880	U881	U882	C883	G884	G885	U886	G887	C888	G889	G890	G891	C892	C893	G894	G895	G896	A897	A898	A899	G900	C901	G902	G903	U904	A905	C906	C907	A908	A909	A910	U911	C912	G913	A914	G915	G916	C917	A918	A919	A920	C921	U922	C923	U924	A927	U928	A929	A932	G933	A934	U935	G936	U937	G938	A939	A940	C941							
A8315	G816	C817	U818	G819	G820	U821	U822	C823	U824	C825	C828	G829	A830	A831	A832	G836	U837	U838	U839	G840	G841	G842	C843	G844	G845	A846	G850	U851	C852	G853	A854	C855	G856	C857	G858	A859	C860	A861	U862	C863	U864	A865	G866	G867	G868	G869	U870	A871	A872	U873	G874	C875	A876	C877	U878	C879								

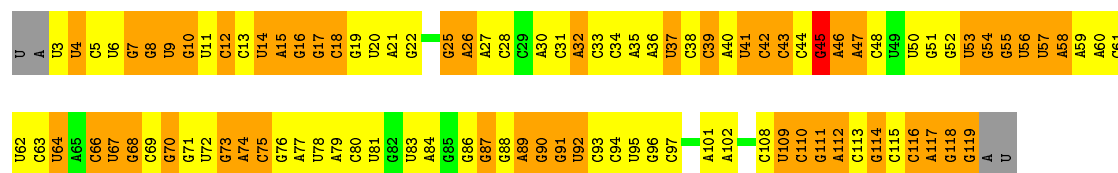


- Molecule 2: Spinach chloroplast 4.5S rRNA



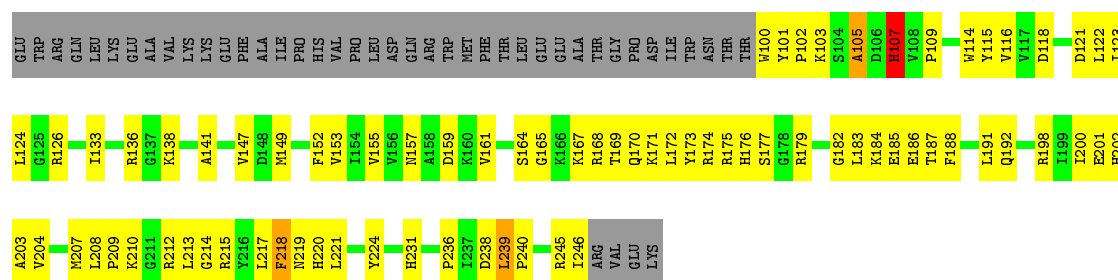
- Molecule 3: 5S rRNA

Chain B:  12% 43% 40% ..



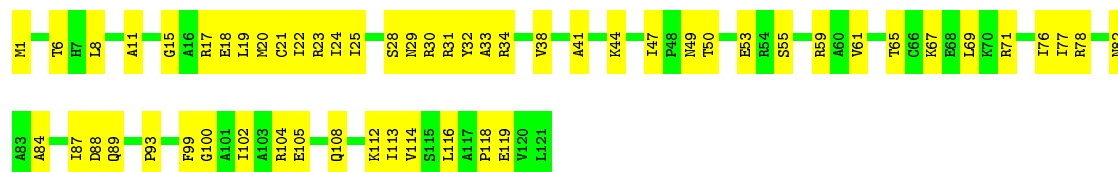
- Molecule 4: 50S ribosomal protein L13, chloroplastic

Chain L: 36% 39% .. 23%



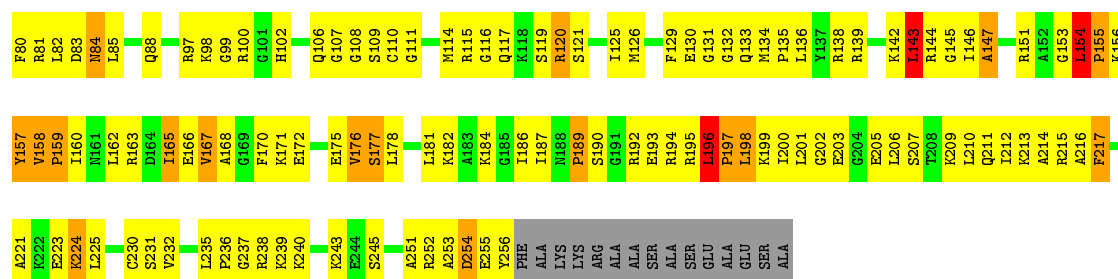
- Molecule 5: 50S ribosomal protein L14, chloroplastic

Chain M:  54% 46%



- Molecule 6: 50S ribosomal protein L15

Chain N: 31% 51% 9% 8%



- Molecule 7: 50S ribosomal protein L16, chloroplastic

Chain O: 44% 54%





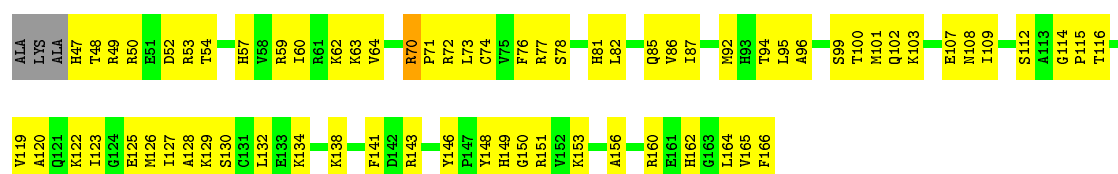
• Molecule 8: 50S ribosomal protein L17

Chain P: 57% 43%



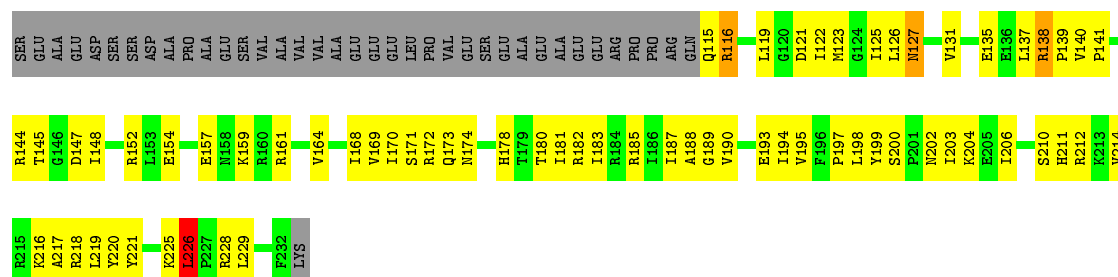
• Molecule 9: 50S ribosomal protein L18

Chain Q: 41% 55% ..



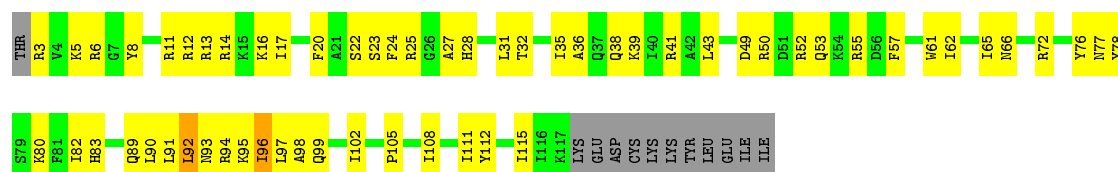
• Molecule 10: 50S ribosomal protein L19, chloroplastic

Chain R: 32% 41% .. 24%



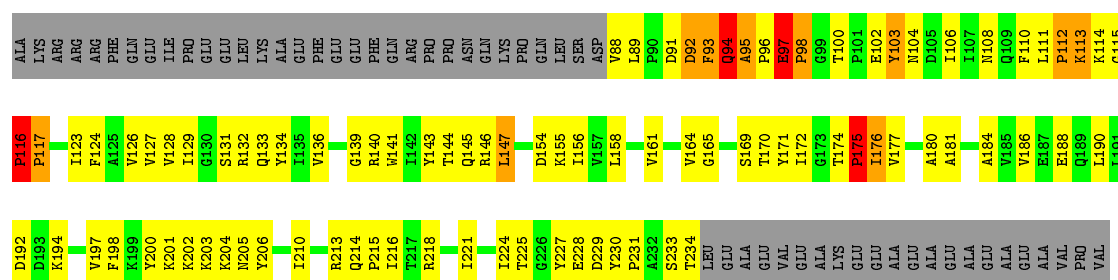
• Molecule 11: 50S ribosomal protein L20, chloroplastic

Chain S: 44% 45% . 9%

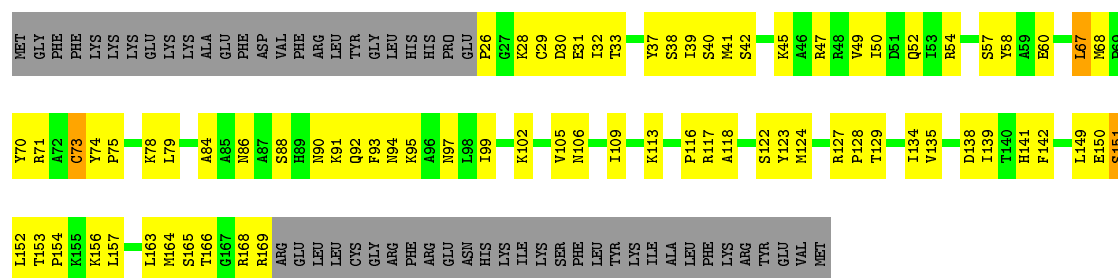


• Molecule 12: 50S ribosomal protein L21, chloroplastic

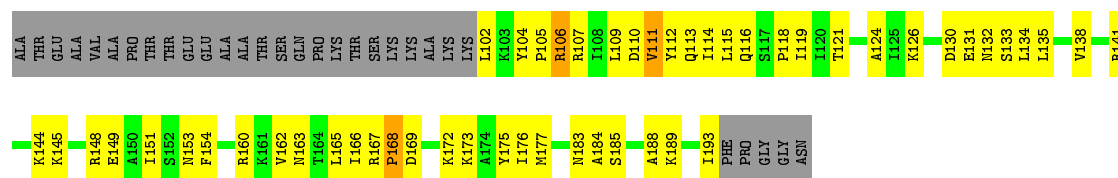
Chain T: 28% 38% 5% . 27%



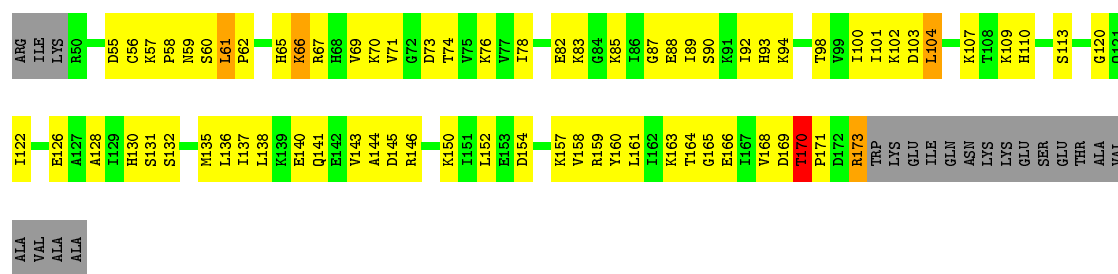
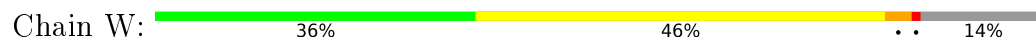
- Molecule 13: 50S ribosomal protein L22, chloroplastic



- Molecule 14: 50S ribosomal protein L23, chloroplastic



- Molecule 15: 50S ribosomal protein L24, chloroplastic



- Molecule 16: 50S ribosomal protein L27

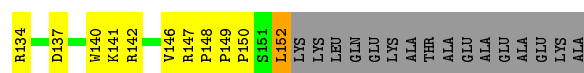
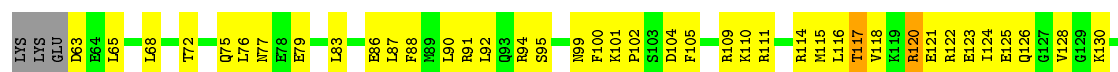




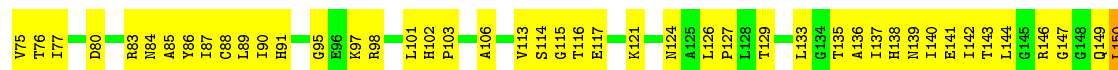
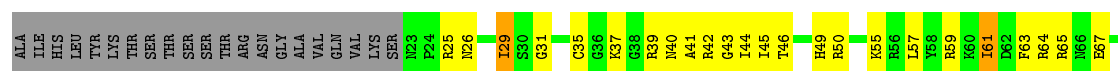
- Molecule 17: 50S ribosomal protein L28



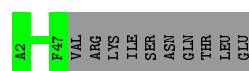
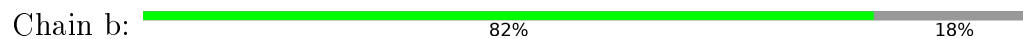
- Molecule 18: 50S ribosomal protein L29



- Molecule 19: 50S ribosomal protein L2, chloroplastic




- Molecule 20: 50S ribosomal protein L32, chloroplastic



- Molecule 21: 50S ribosomal protein L33, chloroplastic




- Molecule 22: 50S ribosomal protein L34, chloroplastic

Chain d: 



- Molecule 23: 50S ribosomal protein L35, chloroplastic

Chain e: 



- Molecule 24: 50S ribosomal protein L36, chloroplastic

Chain f: 



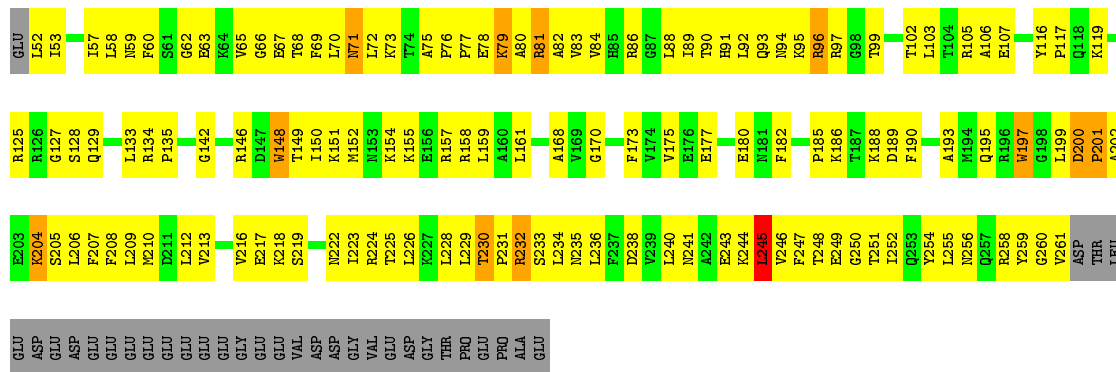
- Molecule 25: 50S ribosomal protein L3

Chain F: 



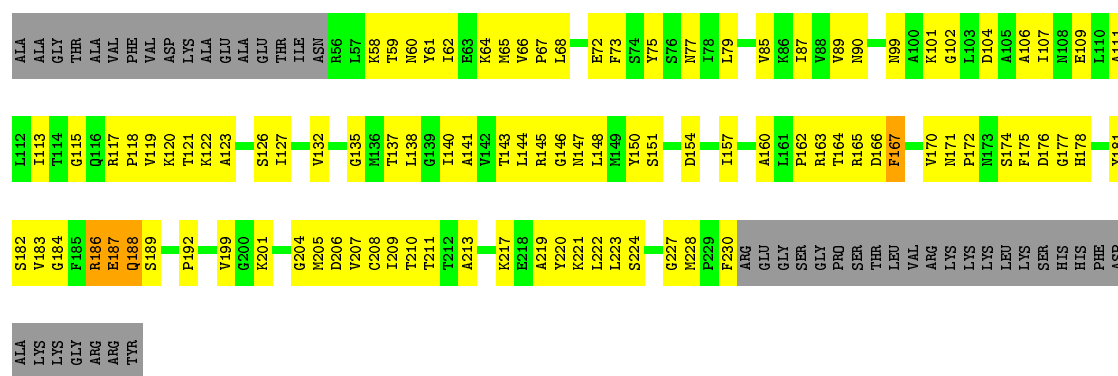
- Molecule 26: 50S ribosomal protein L4, chloroplastic

Chain G: 

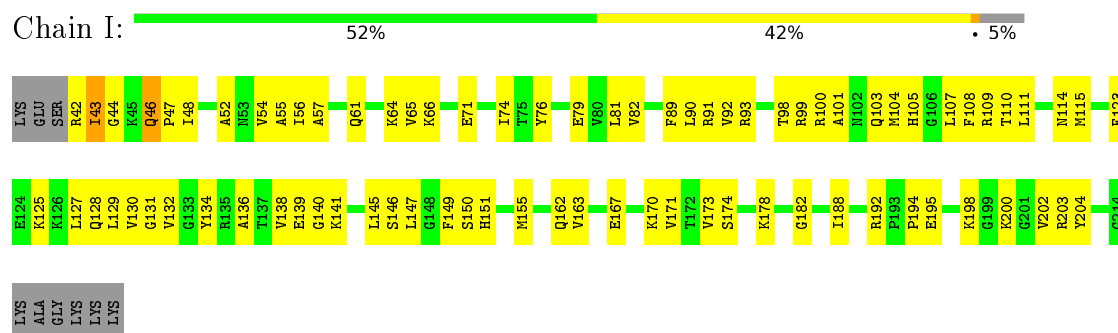


- Molecule 27: 50S ribosomal protein L5, chloroplastic

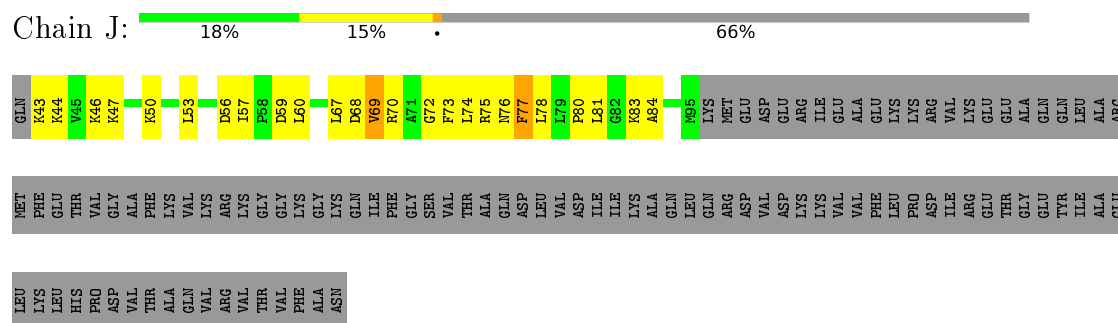
Chain H: 



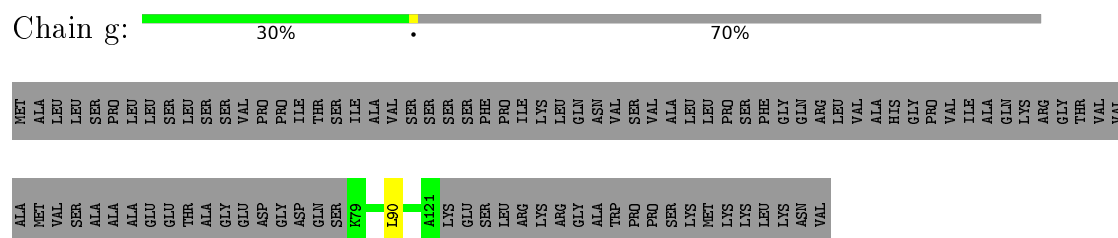
• Molecule 28: 50S ribosomal protein L6



• Molecule 29: 50S ribosomal protein L9



• Molecule 30: 50S ribosomal protein 5 alpha, chloroplastic

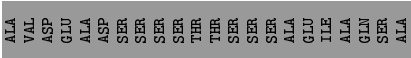


• Molecule 31: 50S ribosomal protein L31





● Molecule 32: 50S ribosomal protein 6, chloroplastic



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	174949	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	109375	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z > 2	RMSZ	# Z > 2
1	A	0.80	18/67340 (0.0%)	0.94	109/105056 (0.1%)
10	R	0.61	0/967	0.79	2/1300 (0.2%)
11	S	0.77	0/1013	0.82	1/1351 (0.1%)
12	T	0.73	0/1199	0.88	3/1633 (0.2%)
13	U	0.60	1/1168 (0.1%)	0.69	0/1566
14	V	0.53	0/749	0.65	0/1006
15	W	0.49	0/1006	0.67	2/1343 (0.1%)
16	X	0.66	0/825	0.80	2/1099 (0.2%)
17	Y	0.65	0/615	0.78	2/819 (0.2%)
18	Z	0.52	0/762	0.71	0/1012
19	E	0.60	0/1938	0.78	1/2603 (0.0%)
2	C	3.05	9/2449 (0.4%)	1.30	26/3817 (0.7%)
20	b	0.72	0/387	0.65	0/513
21	c	0.55	0/422	0.85	1/564 (0.2%)
22	d	0.45	0/447	0.63	0/588
23	e	0.72	0/569	0.82	1/752 (0.1%)
24	f	0.57	0/306	0.78	0/403
25	F	0.66	0/1646	0.74	1/2201 (0.0%)
26	G	0.65	2/1687 (0.1%)	0.78	1/2271 (0.0%)
27	H	0.37	0/1372	0.60	0/1848
28	I	0.49	0/1374	0.63	1/1849 (0.1%)
29	J	0.33	0/427	0.65	0/568
3	B	0.78	0/2796	0.87	2/4357 (0.0%)
30	g	0.44	0/345	0.85	1/455 (0.2%)
31	a	0.29	0/306	0.60	0/413
32	h	0.70	1/382 (0.3%)	0.81	2/520 (0.4%)
4	L	0.67	0/1212	0.68	1/1634 (0.1%)
5	M	0.60	0/951	0.69	1/1282 (0.1%)
6	N	0.40	0/1361	0.77	3/1806 (0.2%)
7	O	0.63	1/1089 (0.1%)	0.71	1/1461 (0.1%)
8	P	0.63	0/959	0.76	0/1280
9	Q	0.52	0/963	0.67	0/1293
All	All	0.88	32/99032 (0.0%)	0.90	164/148663 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	R	0	1
11	S	0	3
13	U	0	1
19	E	0	3
24	f	0	1
25	F	0	1
26	G	0	2
27	H	0	1
32	h	0	2
9	Q	0	1
All	All	0	16

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	95	A	N3-C4	76.76	1.80	1.34
2	C	95	A	C6-N1	71.09	1.85	1.35
2	C	95	A	C5-C4	50.90	1.74	1.38
2	C	95	A	C2-N3	47.29	1.76	1.33
2	C	95	A	N1-C2	47.04	1.76	1.34

The worst 5 of 164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	95	A	N1-C2-N3	-28.24	115.18	129.30
2	C	95	A	C2-N3-C4	24.30	122.75	110.60
2	C	95	A	N7-C8-N9	14.45	121.03	113.80
6	N	196	LEU	C-N-CD	-14.44	88.83	120.60
2	C	95	A	C4-C5-N7	-13.30	104.05	110.70

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	Q	70	ARG	Peptide
10	R	190	VAL	Peptide
11	S	24	PHE	Peptide
11	S	82	ILE	Peptide

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Mol	Chain	Res	Type	Group
11	S	96	ILE	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60117	0	30254	3962	0
2	C	2187	0	1099	306	0
3	B	2500	0	1263	331	0
4	L	1184	0	1221	135	0
5	M	942	0	996	51	0
6	N	1342	0	1413	392	0
7	O	1067	0	1120	103	0
8	P	944	0	1004	68	0
9	Q	947	0	966	87	0
10	R	953	0	1044	80	0
11	S	996	0	1060	122	0
12	T	1171	0	1216	216	0
13	U	1149	0	1220	98	0
14	V	740	0	795	103	0
15	W	993	0	1054	127	0
16	X	810	0	847	185	0
17	Y	605	0	652	51	0
18	Z	754	0	804	99	0
19	E	1904	0	1982	219	0
20	b	378	0	413	0	0
21	c	415	0	434	0	0
22	d	445	0	501	0	0
23	e	563	0	621	0	0
24	f	304	0	342	0	0
25	F	1620	0	1699	174	0
26	G	1655	0	1723	238	0
27	H	1351	0	1407	136	0
28	I	1353	0	1416	90	0
29	J	423	0	488	39	0
30	g	345	0	395	0	0
31	a	300	0	279	0	0
32	h	368	0	386	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	90825	0	60114	6418	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 46.

The worst 5 of 6418 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2351:G:C4	9:Q:64:VAL:HG21	1.27	1.61
2:C:95:A:C6	2:C:95:A:C5	1.79	1.59
16:X:128:TYR:CB	16:X:134:LYS:CD	1.78	1.58
11:S:91:LEU:CD1	12:T:175:PRO:HB3	1.30	1.55
1:A:274:G:C6	1:A:433:C:C6	1.94	1.54

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	145/191 (76%)	120 (83%)	21 (14%)	4 (3%)	6	43
5	M	119/121 (98%)	97 (82%)	22 (18%)	0	100	100
6	N	175/192 (91%)	156 (89%)	6 (3%)	13 (7%)	1	16
7	O	132/135 (98%)	107 (81%)	23 (17%)	2 (2%)	13	56
8	P	114/116 (98%)	96 (84%)	18 (16%)	0	100	100
9	Q	118/123 (96%)	99 (84%)	19 (16%)	0	100	100
10	R	116/156 (74%)	89 (77%)	26 (22%)	1 (1%)	21	68
11	S	113/127 (89%)	91 (80%)	22 (20%)	0	100	100
12	T	145/201 (72%)	108 (74%)	28 (19%)	9 (6%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	U	142/199 (71%)	117 (82%)	24 (17%)	1 (1%)	26	72
14	V	90/122 (74%)	79 (88%)	9 (10%)	2 (2%)	8	49
15	W	122/145 (84%)	95 (78%)	25 (20%)	2 (2%)	12	55
16	X	98/137 (72%)	87 (89%)	7 (7%)	4 (4%)	3	33
17	Y	72/77 (94%)	61 (85%)	11 (15%)	0	100	100
18	Z	88/109 (81%)	85 (97%)	3 (3%)	0	100	100
19	E	245/271 (90%)	187 (76%)	57 (23%)	1 (0%)	39	81
20	b	44/56 (79%)	35 (80%)	9 (20%)	0	100	100
21	c	49/65 (75%)	34 (69%)	15 (31%)	0	100	100
22	d	55/60 (92%)	47 (86%)	6 (11%)	2 (4%)	4	37
23	e	67/73 (92%)	50 (75%)	16 (24%)	1 (2%)	13	56
24	f	35/37 (95%)	30 (86%)	5 (14%)	0	100	100
25	F	210/221 (95%)	173 (82%)	37 (18%)	0	100	100
26	G	208/243 (86%)	166 (80%)	40 (19%)	2 (1%)	19	66
27	H	173/220 (79%)	145 (84%)	27 (16%)	1 (1%)	30	75
28	I	171/182 (94%)	142 (83%)	27 (16%)	2 (1%)	16	61
29	J	51/155 (33%)	41 (80%)	9 (18%)	1 (2%)	9	51
30	g	41/142 (29%)	36 (88%)	5 (12%)	0	100	100
31	a	36/94 (38%)	26 (72%)	9 (25%)	1 (3%)	6	43
32	h	44/116 (38%)	31 (70%)	12 (27%)	1 (2%)	8	48
All	All	3218/4086 (79%)	2630 (82%)	538 (17%)	50 (2%)	17	55

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	107	HIS
6	N	143	LEU
6	N	147	ALA
6	N	154	LEU
6	N	155	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	125/165 (76%)	124 (99%)	1 (1%)	86	95
5	M	101/101 (100%)	101 (100%)	0	100	100
6	N	135/144 (94%)	126 (93%)	9 (7%)	20	61
7	O	107/108 (99%)	107 (100%)	0	100	100
8	P	96/96 (100%)	96 (100%)	0	100	100
9	Q	99/100 (99%)	99 (100%)	0	100	100
10	R	104/135 (77%)	101 (97%)	3 (3%)	50	81
11	S	102/114 (90%)	102 (100%)	0	100	100
12	T	129/174 (74%)	122 (95%)	7 (5%)	27	67
13	U	126/176 (72%)	125 (99%)	1 (1%)	86	95
14	V	81/103 (79%)	80 (99%)	1 (1%)	78	92
15	W	112/129 (87%)	109 (97%)	3 (3%)	52	83
16	X	85/111 (77%)	74 (87%)	11 (13%)	5	27
17	Y	64/67 (96%)	61 (95%)	3 (5%)	32	72
18	Z	83/97 (86%)	79 (95%)	4 (5%)	31	71
19	E	195/216 (90%)	189 (97%)	6 (3%)	47	81
20	b	39/49 (80%)	39 (100%)	0	100	100
21	c	48/59 (81%)	47 (98%)	1 (2%)	61	86
22	d	47/49 (96%)	45 (96%)	2 (4%)	35	74
23	e	59/62 (95%)	58 (98%)	1 (2%)	68	89
24	f	34/34 (100%)	34 (100%)	0	100	100
25	F	174/182 (96%)	170 (98%)	4 (2%)	58	85
26	G	176/205 (86%)	169 (96%)	7 (4%)	38	75
27	H	148/183 (81%)	146 (99%)	2 (1%)	74	91
28	I	147/154 (96%)	147 (100%)	0	100	100
29	J	47/134 (35%)	46 (98%)	1 (2%)	61	86
30	g	39/121 (32%)	39 (100%)	0	100	100
31	a	33/83 (40%)	32 (97%)	1 (3%)	48	81
32	h	40/96 (42%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2775/3447 (80%)	2707 (98%)	68 (2%)	59 84

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	X	146	ASN
17	Y	131	LYS
26	G	232	ARG
16	X	150	TYR
16	X	162	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
15	W	68	HIS
18	Z	77	ASN
26	G	257	GLN
15	W	121	GLN
15	W	133	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2796/2810 (99%)	962 (34%)	106 (3%)
2	C	101/106 (95%)	45 (44%)	4 (3%)
3	B	116/121 (95%)	54 (46%)	5 (4%)
All	All	3013/3037 (99%)	1061 (35%)	115 (3%)

5 of 1061 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	C
1	A	13	A
1	A	22	G
1	A	27	A
1	A	32	U

5 of 115 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1254	U
1	A	1531	A
2	C	29	U
1	A	1256	G
1	A	1341	C

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.